

Highly accurate calculation of the resonances in the Stark effect in hydrogen

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Abstract

We obtained accurate resonances for the Stark effect in hydrogen by means of three independent methods. Two of them are based on complex rotation of the coordinates and diagonalization of the Hamiltonian matrix (CRLM and CRCH). The other one is based on the Riccati equations for the logarithmic derivatives of factors of the wavefunction (RPM). The latter approach enabled us to obtain the most accurate results and extremely sharp resonances.

1 Introduction

The Stark effect in hydrogen is an old problem in atomic spectroscopy and one of the first triumphs of wave mechanics [1, 2] (and references therein). The Schrödinger equation is separable in parabolic and squared parabolic coordinates which facilitates the application of most approximate methods [2].

In a recent paper Fernández-Menchero and Summers [3] obtained the complex eigenvalues and eigenfunctions of the Hamiltonian operator for the hydrogen

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atom in a uniform electric field. They resorted to the Lagrange-mesh basis set, proposed by Lin and Ho [4] for the treatment of the Yukawa potential in a uniform electric field, and the complex-rotation method [5]. They compared their results with those obtained by Lin and Ho [4], Kolosov [6], Rao and Li [7] and Ivanov [8] and overlooked the earlier impressive calculations of Benassi and Grecchi [9] and the accurate results obtained by Fernández [10]. Benassi and Grecchi resorted to complex scaling and a basis set of confluent hypergeometric functions that is suitable when the Schrödinger equation is written in squared parabolic coordinates. On the other hand, Fernández applied the straightforward Riccati-Padé method (RPM) that does not require the use of complex coordinates.

The purpose of this paper is to calculate the Stark resonances as accurately as possible by means of the methods proposed by Fernández-Menchero and Summers [3], Benassi and Grecchi [9] and Fernández [10] and compare the results with those obtained by the authors already mentioned and also by Damburg and Kolosov [11]. There is a vast literature on the hydrogen atom in a uniform electric field but we restrict present discussion to some of the available calculations that we deem are suitable for comparison.

In section 2 we outline the main ideas about separating the Schrödinger equation in parabolic and squared parabolic coordinates. In sections 3, 4 and 5 we briefly introduce the methods of Fernández-Menchero and Summers [3], Benassi and Grecchi [9] and the RPM [10], respectively. In section 6 we compare the results of various approaches and in section 7 we summarize the main results and draw conclusions.

2 Stark effect in hydrogen

The Schrödinger equation in atomic units is

$$\begin{aligned}
H\psi &= E\psi \\
H &= -\frac{1}{2}\nabla^2 - \frac{1}{r} + Fz,
\end{aligned} \tag{1}$$

where F is the intensity of the uniform electric field assumed to be directed along the z axis.

This equation is separable in parabolic coordinates

$$\begin{aligned}
x &= \sqrt{\xi\eta} \cos \phi, \quad y = \sqrt{\xi\eta} \sin \phi, \quad z = \frac{\xi - \eta}{2} \\
\xi &\geq 0, \quad \eta \geq 0, \quad 0 \leq \phi \leq 2\pi.
\end{aligned} \tag{2}$$

If we write

$$\psi(x, y, z) = (\xi\eta)^{-1/2} u(\xi) v(\eta) e^{im\phi}, \quad m = 0, \pm 1, \pm 2, \dots, \tag{3}$$

then we obtain two equations of the form

$$\left(\frac{d^2}{dx^2} + \frac{1 - m^2}{4x^2} + \frac{E}{2} - \sigma \frac{F}{4} x + \frac{A_\sigma}{x} \right) \Phi(x) = 0, \tag{4}$$

where $\sigma = \pm 1$ and $A_+ = A$ and $A_- = 1 - A$ are separation constants. When $\sigma = 1$, $x = \xi$ and $\Phi(\xi) = u(\xi)$; when $\sigma = -1$, $x = \eta$ and $\Phi(\eta) = v(\eta)$.

The Schrödinger equation (1) is also separable in squared parabolic coordinates

$$\begin{aligned}
x &= \mu\nu \cos \phi, \quad y = \mu\nu \sin \phi, \quad z = \frac{\mu^2 - \nu^2}{2} \\
\mu &\geq 0, \quad \nu \geq 0, \quad 0 \leq \phi \leq 2\pi.
\end{aligned} \tag{5}$$

If in this case we write

$$\psi(x, y, z) = (\mu\nu)^{-1/2} u(\mu) v(\nu) e^{im\phi}, \tag{6}$$

then we obtain two equations of the form

$$\left(\frac{d^2}{dx^2} + \frac{1 - 4m^2}{4x^2} + 2Ex^2 - \sigma Fx^4 + Z_\sigma \right) \Phi(x) = 0, \quad (7)$$

where, $\sigma = \pm 1$ and $Z_+ = Z$ and $Z_- = 4 - Z$ are the separation constants. When $\sigma = 1$, $x = \mu$ and $\Phi(\mu) = u(\mu)$; when $\sigma = -1$, $x = \nu$ and $\Phi(\nu) = v(\nu)$.

The solutions to the equations in either set of coordinates are commonly labelled by the quantum numbers $n_1, n_2 = 0, 1, 2 \dots$ and $m = 0, 1, \dots$, and the notation $|n_1, n_2, m\rangle$ is suitable for referring to them. We will sometimes resort to the principal quantum number $n = n_1 + n_2 + |m| + 1$ to denote a set of states. Obviously, m is the only good quantum number; the other ones refer to the states of the hydrogen atom and are valid when $F = 0$.

3 Complex rotation and Laguerre-mesh basis set

Fernández-Menchero and Summers [3] decided to treat the Schrödinger equation as nonseparable. The Hamiltonian operator in parabolic coordinates reads

$$H = -\frac{2}{\xi + \eta} \left[\frac{\partial}{\partial \xi} \left(\xi \frac{\partial}{\partial \xi} \right) + \frac{\partial}{\partial \eta} \left(\eta \frac{\partial}{\partial \eta} \right) \right] - \frac{1}{2\xi\eta} \frac{\partial^2}{\partial \phi^2} - \frac{2}{\xi + \eta} + F \frac{\xi - \eta}{2}, \quad (8)$$

and the authors proposed the variational ansatz

$$\psi(\xi, \eta, \phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \sum_{k=1}^N \sum_{l=1}^N c_{klm} e^{-\frac{\xi+\eta}{2}} (\xi\eta)^{\frac{|m|}{2}} \Lambda_{Nk}(\xi) \Lambda_{Nl}(\eta) \quad (9)$$

$$\Lambda_{Nk}(x) = (-1)^k \sqrt{x_k} \frac{L_N(x)}{x - x_k}, \quad (10)$$

where $L_N(x)$ is the Laguerre polynomial of degree N and x_k its k -th zero. In order to obtain the resonances they resorted to the well-known complex rotation method [5] that in this case is given by the transformation $(\xi, \eta) \rightarrow (e^{i\vartheta}\xi, e^{i\vartheta}\eta)$, where ϑ is the rotation angle. The eigenvalues and expansion coefficients are

given by the secular equation

$$(\mathbf{H} - E\mathbf{S})\mathbf{C} = 0, \quad (11)$$

where the elements of the $N^2 \times N^2$ matrices \mathbf{H} and \mathbf{S} are explicitly shown elsewhere [3] and the elements of the column vector \mathbf{C} are the coefficients c_{klm} . Note that the integrals appearing in the matrix elements of both \mathbf{H} and \mathbf{S} should be calculated numerically and when we increase N we have to calculate all those integrals again. For brevity we will call this method CRLM.

4 Complex scaling and confluent hypergeometric basis set

In order to obtain the resonances Benassi and Grecchi [9] resorted to equation (7) and a basis set of the form

$$\varphi_{m,n}(x) = \frac{2(m+n)!}{m!n!} e^{-x^2/2} x^{m+\frac{1}{2}} F(-n, m+1; x^2), \quad (12)$$

where $F(a, b, z)$ is the confluent hypergeometric function. In this case the authors resorted to the complex scaling method that is based on the transformation $(\mu, \nu) \rightarrow (\lambda^{1/2}\mu, \lambda^{1/2}\nu)$, where λ is a complex number. The complex scaling method contains the complex rotation method as a particular case because $\lambda = |\lambda|e^{i\vartheta}$ and the proper choice of $|\lambda|$ enables one to improve the convergence of the approach.

In this case all the elements of the relevant pentadiagonal matrix can be calculated analytically and are independent of the matrix dimension. This approach will be called CRCH from now on.

5 The Riccati-Padé method

We can apply the RPM to the eigenvalue equations derived in either parabolic or squared parabolic coordinates. In the earlier application of the approach Fernández [10] chose the former and here we resort to the latter. It is worth mentioning that the performance of the RPM in both sets of coordinates is identical and that the reason for the selection of the squared parabolic coordinates is to have a closer contact between the RPM and the CRCH method of Benassi and Grecchi [9]. The regularized logarithmic derivative

$$f(x) = \frac{s}{x} - \frac{\Phi'(x)}{\Phi(x)}, \quad s = |m| + \frac{1}{2}, \quad (13)$$

can be expanded in a Taylor series

$$f(x) = \sum_{j=0}^{\infty} f_j x^{2j+1}, \quad (14)$$

where the coefficients f_j are polynomial functions of E and Z . The details of the method are outlined elsewhere [10]; here it suffices to say that we construct Hankel determinants of the form

$$H_D^d(E, Z, F) = \begin{vmatrix} f_{d+1} & f_{d+2} & \cdots & f_{D+d} \\ f_{d+2} & f_{d+3} & \cdots & f_{D+d+1} \\ & & \ddots & \\ f_{D+d} & f_{D+d+1} & \cdots & f_{2D+d-1} \end{vmatrix}, \quad (15)$$

and obtain the approximate eigenvalues $E^{[D,d]}$ from the roots of the set of nonlinear equations

$$H_D^d(E, Z, F) = H_D^d(E, 4 - Z, -F) = 0. \quad (16)$$

The main advantage of the RPM is the enormous rate of convergence which enables us to obtain very accurate eigenvalues with determinants of relatively small dimension. However, the great number of roots in the neighborhood of each eigenvalue makes it difficult to find the optimal sequence that converges to it. Since we resort to the Newton-Raphson algorithm to obtain the roots of the system of equations (16) we have to choose the starting point quite close to the chosen root. We will discuss this point briefly in Section 6. The RPM is most suitable for the treatment of separable problems.

6 Numerical calculations

In order to apply the CRLM [3] we calculated all the integrals numerically with a tolerance of 10^{-15} . For each value of F , m and N we varied the rotation angle ϑ between 0.3 and 0.7 looking for those eigenvalues that remained almost constant. We could reproduce the results in the literature with matrices of dimension $N = 30$ [12].

The only exact quantum number is m , however, it is customary to resort to the quantum numbers of the isolated hydrogen atom in order to label the energies and states of the Stark problem. Some authors choose the parabolic quantum numbers $n_1, n_2 = 0, 1, 2, \dots$ [9] and others the principal quantum number $n = n_1 + n_2 + |m| + 1$ and $k = n_1 - n_2$ [3].

In the case of CRCH we first solved the eigenvalue equations that yield the eigenvalues Z_+ and Z_- and then applied the Newton-Raphson method to solve the equation $Z_+ + Z_- - 4 = 0$. Details of the calculation are given elsewhere [9]; we just mention that in order to obtain a starting point for the Newton-Raphson method we resorted to the results provided by perturbation theory [16].

The Hankel determinants that appear in the RPM are polynomial functions of E and Z of great degree. For this reason it is necessary to handle complex numbers with sufficiently great precision and we resorted to the GNU MPC library [13]. The Hankel determinants can be calculated numerically by means of the well known recurrence relation

$$H_D^d = \frac{H_{D-1}^d H_{D-1}^{d+2} - (H_{D-1}^{d+1})^2}{H_{D-2}^{d+2}} \quad (17)$$

with the initial conditions $H_0^d = 1$ and $H_1^d = f_{d+1}$. Once we calculate the desired determinants we obtain the eigenvalue and separation constant by means of the Newton-Raphson method. In order to have a suitable starting point we resorted to CRCH results.

The remarkable rate of convergence of the RPM is clearly illustrated by the calculation of the logarithmic error $\log |\alpha^{[D]} - \alpha^{[D-1]}|$ where α stands for either $\text{Re}E$ or $\text{Im}E$. We do not indicate the value of d explicitly because in present calculations we have chosen $d = 0$. Figures 1 and 2 show the logarithmic error for all the resonances with $n = 1, 2, \dots, 6$ and field strengths $F = 0.001$ and $F = 0.005$, respectively. As the quantum numbers increase the minimum value of D at which the resonance appears also increases. For example, the lowest resonance appears as a root of the Hankel determinant with $D = 2$ and $|0, 5, 0\rangle$ appears at $D = 11$. The rate of convergence is greater when the root of the Hankel determinant is real. This fact is clearly shown in Fig. 2 where the imaginary part of $|0, 0, 0\rangle$ appears at $D = 22$. When $F = 0.001$ the imaginary part of the lowest resonance appears at $D = 103$ which is the reason why the rate of convergence for this resonance is considerably greater than the other ones for all $D \leq 100$. When $D > 103$ the rate of convergence for the lowest resonance becomes similar to the other ones.

The resonances explicitly labelled in figures 1 and 2 are shown in Table 1 with their number of digits truncated to a reasonable size.

Figure 3 shows that our estimated value of $\text{Im}E$ for the lowest resonance is in perfect agreement with the analytic asymptotic formula derived by Benassi and Grecchi [9]:

$$|\text{Im}E| \sim 2F^{-1}e^{-2/(3F)} \left(1 - 8.916F + 25.57F^2 + O(F^3)\right). \quad (18)$$

The RPM is also suitable for the calculation of higher resonances. For example, tables 2 and 3 compare present results obtained by the CRCH and RPM for two states with $n = 5$ with those obtained earlier by Damburg and Kolosov [11]. Table 4 compares present RPM results for some states with $n = 10$ with those obtained by Kolosov [6]. The discrepancy in the imaginary part for the case $|0, 9, 0\rangle$, $F = 2.2 \times 10^{-5}$, is probably due to a misprint in that reference. Table 5 shows the resonance $|39, 0, 0\rangle$ for several values of the field strength. We do not compare these results with those of Kolosov [6] because he did not indicate the conversion factor from atomic units to $V\text{cm}^{-1}$ shown in his table. However, Fig. 4 shows that both sets of results are in reasonable agreement.

In the tables discussed above we have truncated present RPM results to a reasonable number of digits. We have obtained them with much higher accuracy as suggested by figures 1 and 2. For example, for the lowest resonance and field strength $F = 0.005$ we obtained

$$\begin{aligned} \text{Re}E &= -0.50005628479379296933177394769143288196325092731889137262135731 \\ &\quad 28725736315548994436307340293823812601699152241599625041068943791 \\ &\quad 42099665225189334039046848974164185728077545219665133771938893895 \\ &\quad 64251327341968732189236225621425838831553440690618168917215735013 \\ &\quad 803880912033036 \\ \text{Im}E &= -4.74901370837102040886757127120827250441845432417751748825418970 \\ &\quad 22400488040285011762035775189238632536585799373474503067879411046 \\ &\quad 22147574080708907330396144467615023762954201754322979890803189455 \\ &\quad 51562966634796276868224 \times 10^{-56} \end{aligned} \quad (19)$$

with Hankel determinants of dimension $D \leq 150$. In principle we expect that a properly truncated perturbation series will exhibit an accuracy of the order of

$|\text{Im}E|$. On summing the first 130 terms of the perturbation series calculated by means of the hypervirial perturbative method [16] we obtained the following result:

$$E^{PT} = -0.5000562847937929693317739476914328819632509273188913726, \quad (20)$$

that agrees with the RPM one to the last digit. It is not easy to obtain such a sharp resonance by means of other approaches; for example, Fernández-Menchero and Summers [3] estimated $\text{Re}E = -0.5000553416$ and $\text{Im}E = 0.8944475605 \times 10^{-7}$. We calculated the real part of this resonance more accurately by means of the CRLM but were unable to obtain a reasonable estimate of the imaginary part [12].

The RPM enables one to calculate even sharper resonances; for example, for the lowest one and $F = 0.001$ we obtained

$$\begin{aligned} \text{Re}E &= -0.50000225005555178356591589970608204532866714376652965654995937 \\ &\quad 97019283545891048870035463753481536961447568150634794700138591827 \\ &\quad 91549628581187487453336046428670620173909589867079695807271725700 \\ &\quad 47474205292728633151353049600188535220623998127315129221076077663 \\ &\quad 756392409425470889188167975544640438386213612059475282765271923 \\ \text{Im}E &= -5.854592875137598393486482622915575 \times 10^{-287} \end{aligned} \quad (21)$$

with Hankel determinants of dimension $D \leq 130$. In this case perturbation theory of order 600 (300 nonzero terms) yields

$$\begin{aligned} E^{PT} &= -0.50000225005555178356591589970608204532866714376652965654995937970 \\ &\quad 19283545891048870035463753481536961447568150634794700138591827915496 \\ &\quad 28581187487453336046428670620173909589867079695807271725700474742052 \\ &\quad 92728633151353049600188535220623998127315129221076077663756392409425 \\ &\quad 47088918816797549 \end{aligned} \quad (22)$$

7 Conclusions

We have calculated the resonances of the Stark effect in hydrogen by means of three independent methods. Although we were able to improve the CRLM calculation considerably [12] we think that the CRCH is far more efficient. However, the RPM yielded considerable more accurate results and enabled us to obtain extremely sharp resonances that we were not able to obtain by means of the other two methods. The reason is that the accuracy of the real part should be at least of the order of the imaginary one. We were able to attain such an accuracy in the calculation of the roots of the RPM equations (16) thanks to the GNU MPC library [13]. We think that it is almost impossible to do the same by means of the CRLM because of the numerical calculation of the matrix elements. In principle, one can obtain the resonances with any degree of accuracy by means of the CRCH but such calculation would require a great deal of ingenuity. For this reason we think that the RPM is an extremely suitable benchmark to test other approaches on separable models.

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Table 1

Resonances for the states appearing in figures 1 and 2

F	Resonance	$\text{Re}(E)$	$\text{Im}(E)$
0.001	$ 0, 0, 0\rangle$	-0.5000022500555518	$-6.584169959231863 \times 10^{-287}$
	$ 0, 0, 1\rangle$	-0.1250782240371032	$-8.433615180808857 \times 10^{-33}$
	$ 0, 1, 0\rangle$	-0.1280858350607099	$-2.060525710039887 \times 10^{-31}$
	$ 1, 0, 0\rangle$	-0.1220826861326878	$-3.395926205766083 \times 10^{-34}$
	$ 0, 5, 0\rangle$	-0.05215538955477732	$-2.594493723108199 \times 10^{-2}$
0.005	$ 0, 0, 0\rangle$	-0.5000562847937930	$-4.749013708371020 \times 10^{-56}$
	$ 0, 0, 1\rangle$	-0.1271466127039709	$-1.307642723230557 \times 10^{-5}$
	$ 0, 1, 0\rangle$	-0.1426186075727077	$-5.297223183652474 \times 10^{-5}$
	$ 1, 0, 0\rangle$	-0.1120619240019938	$-2.864684219868783 \times 10^{-6}$
	$ 0, 5, 0\rangle$	-0.1213596730003857	$-1.176260968442979 \times 10^{-1}$

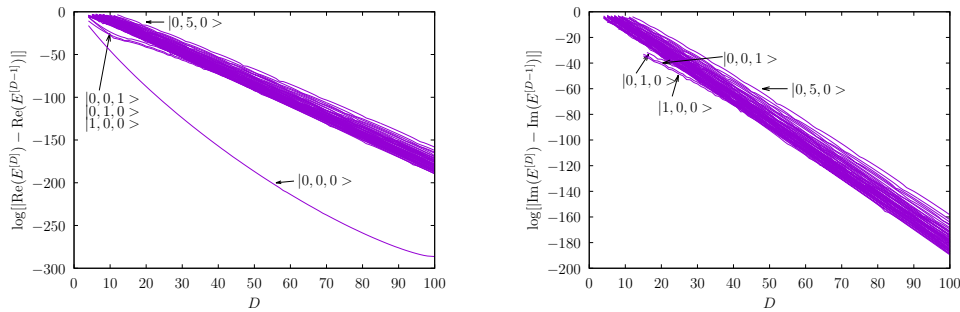
Fig. 1. Convergence of the RPM resonances for $F = 0.001$ 

Table 2

Resonance $|0, 4, 0\rangle$ from reference [11] (a) and present calculation by means of CRCH

(b) and RPM (c)

F		$\text{Re}(E)$	$\text{Im}(E)$
0.00010	a	-0.0231791962	-2.1×10^{-12}
	b	-0.02317919625030	-2.1135×10^{-12}
	c	-0.02317919625030518	$-2.113884073268850 \times 10^{-12}$
0.00015	a	-0.024956749	-9.595×10^{-7}
	b	-0.024956750918078	$-9.6007202913 \times 10^{-7}$
	c	-0.02495675091807878	$-9.600720291331372 \times 10^{-7}$
0.00020	a	-0.02697136	-8.9150×10^{-5}
	b	-0.0269800814710915	$-9.36280360832384 \times 10^{-5}$
	c	-0.02698008147109154	$-9.362803608323849 \times 10^{-5}$
0.00025	a	-0.02896828	-4.2655×10^{-4}
	b	-0.02912946983310681	$-4.868994650393436 \times 10^{-4}$
	c	-0.02912946983310681	$-4.868994650393436 \times 10^{-4}$
0.00030	a	-0.0305381	-9.849×10^{-4}
	b	-0.03122955458572655	$-1.127494087615666 \times 10^{-3}$
	c	-0.03122955458572655	$-1.127494087615666 \times 10^{-3}$
0.00035	a	-0.0314338	-1.8217×10^{-3}
	b	-0.03323652729915596	$-1.945324601526496 \times 10^{-3}$
	c	-0.03323652729915596	$-1.945324601526496 \times 10^{-3}$
0.00040	a	-0.031408	-3.17565×10^{-3}
	b	-0.03512209724011620	$-2.892832253491630 \times 10^{-3}$
	c	-0.03512209724011620	$-2.892832253491630 \times 10^{-3}$
0.00045	a	-0.02998	-6.365×10^{-3}
	b	-0.03687445248862566	$-3.911655467856354 \times 10^{-3}$
	c	-0.03687445248862566	$-3.911655467856354 \times 10^{-3}$

Table 3

Resonances for the state $|4, 0, 0\rangle$ from reference [11] (a) and present calculation by means of CRCH (b) and RPM (c)

F		$\text{Re}(E)$	$\text{Im}(E)$
0.00015	a	-0.0158077645	-1×10^{-11}
	b	-0.01580776440749585	$-7.156147028941416 \times 10^{-12}$
	c	-0.01580776440749585	$-7.156147028941416 \times 10^{-12}$
0.00020	a	-0.0145352049	-2.013-8
	b	-0.01453520517676726	$-2.012419057345574 \times 10^{-8}$
	c	-0.01453520517676726	$-2.012419057345574 \times 10^{-8}$
0.00025	a	-0.013328925	-1.63595×10^{-6}
	b	-0.01332892813256598	$-1.637235677233378 \times 10^{-6}$
	c	-0.01332892813256598	$-1.637235677233378 \times 10^{-6}$
0.00030	a	-0.01220093	-2.0833×10^{-5}
	b	-0.01220135935615766	$-2.104916128829678 \times 10^{-5}$
	c	-0.01220135935615766	$-2.104916128829678 \times 10^{-5}$
0.00035	a	-0.01113604	-8.9570×10^{-5}
	b	-0.01114288854595917	$-9.327043407081445 \times 10^{-5}$
	c	-0.01114288854595917	$-9.327043407081445 \times 10^{-5}$
0.00040	a	-0.01008206	-2.1402×10^{-4}
	b	-0.01011729953739499	$-2.321591626792999 \times 10^{-4}$
	c	-0.01011729953739499	$-2.321591626792999 \times 10^{-4}$
0.00045	a	-0.00899479	-3.7941×10^{-4}
	b	-0.00909725070184054	$-4.263615594700631 \times 10^{-4}$
	c	-0.00909725070184054	$-4.263615594700631 \times 10^{-4}$
0.00050	a	-0.0078517	-5.7415×10^{-4}
	b	-0.00807076238659657	$-6.601708601710509 \times 10^{-4}$
	c	-0.00807076238659657	$-6.601708601710509 \times 10^{-4}$

Table 4

Resonances calculated by Kolosov [6] (a) and by means of the RPM with $D = 30$

(b)

 $|9, 0, 0\rangle$

$10^5 F$		Re E	Im E
2.0	a	$-2.58557398 \times 10^{-3}$	-9.509227×10^{-8}
	b	$-2.585573979364734 \times 10^{-3}$	$-9.509226978683682 \times 10^{-8}$
3.0	a	$-1.57105982 \times 10^{-3}$	-3.959433×10^{-5}
	b	$-1.571059822031523 \times 10^{-3}$	$-3.959432995212450 \times 10^{-5}$
4.0	a	$-5.8496223 \times 10^{-4}$	$-1.6703408 \times 10^{-4}$
	b	$-5.849621042229387 \times 10^{-4}$	$-1.670340346132577 \times 10^{-4}$

 $|0, 0, 9\rangle$

$10^5 F$		Re E	Im E
2.0	a	$-5.32440479 \times 10^{-3}$	$-3.9351431 \times 10^{-5}$
	b	$-5.324404794258087 \times 10^{-3}$	$-3.935143048784509 \times 10^{-5}$
3.0	a	$-5.6483507 \times 10^{-3}$	-3.263613×10^{-4}
	b	$-5.648350339949772 \times 10^{-3}$	$-3.263623549768137 \times 10^{-4}$

 $|0, 9, 0\rangle$

$10^5 F$		Re E	Im E
1.4	a	$-7.2120845 \times 10^{-3}$	$-4.0070215 \times 10^{-5}$
	b	$-7.212084472616482 \times 10^{-3}$	$-4.007021552503371 \times 10^{-5}$
1.8	a	-7.977367×10^{-3}	$-2.4391785 \times 10^{-4}$
	b	$-7.977367228278029 \times 10^{-3}$	$-2.439179991742931 \times 10^{-4}$
2.2	a	-8.660578×10^{-3}	-5.32992×10^{-6}
	b	$-8.660579416493959 \times 10^{-3}$	$-5.329919686471733 \times 10^{-4}$

Table 5

Resonance $|39, 0, 0\rangle$ calculated by means of the RPM with $D \leq 65$

$10^7 F$	$\text{Re}E$	$\text{Im}E$
1.0	$-1.033131815036742 \times 10^{-4}$	$-1.410563208376528 \times 10^{-12}$
1.2	$-6.597779434524293 \times 10^{-4}$	$-2.882918724695370 \times 10^{-8}$
1.4	$-3.007626411426787 \times 10^{-5}$	$-8.858397640808244 \times 10^{-7}$
1.6	$5.730328096956075 \times 10^{-6}$	$-2.598217010741238 \times 10^{-6}$
1.8	$4.153413722356150 \times 10^{-5}$	$-4.277370190378267 \times 10^{-6}$
2.0	$7.701721282910781 \times 10^{-5}$	$-5.720318291587286 \times 10^{-6}$
2.2	$1.120415206875958 \times 10^{-4}$	$-6.975702947269457 \times 10^{-6}$

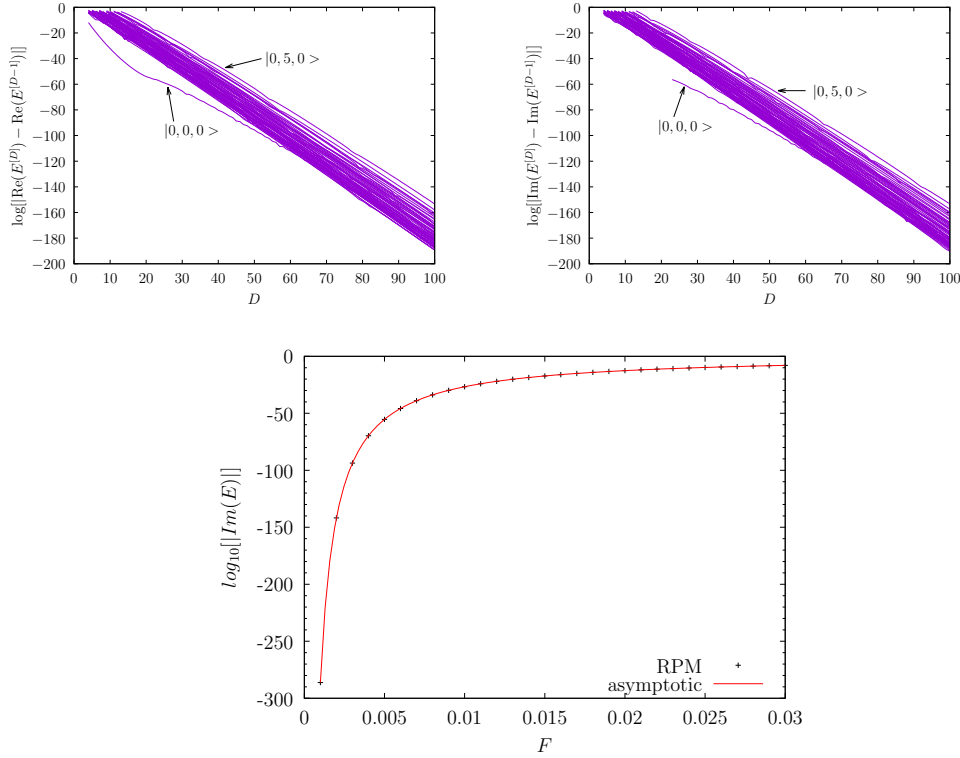
Fig. 2. Convergence of the RPM resonances for $F = 0.005$ 

Fig. 3. Width of the lowest resonance calculated by means of the RPM (circles) and the asymptotic expansion (18) (line)

Fig. 4. Real and imaginary parts of the resonance $|39, 0, 0\rangle$: (a) [6], (b) RPM

